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ARKIV FÖR KEMI Band 5 nr 4

Communicated 14 May 1952 by ARNE WESTGREN

The structure of $\text{Bi}_2\text{NbO}_5\text{F}$ and isomorphous compounds

By BENGT AURIVILLIUS

With 1 figure in the text

X-ray studies made previously on the compounds $\text{CaBi}_2\text{Nb}_2\text{O}_9$, $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ and $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ (1) showed that they have very similar structures. The symmetry is tetragonal or pseudotetragonal, and the structures are each built up of quadratic Bi_2O_2 layers alternating with perovskite layers, the latter having different heights in the three different cases. The generalized formula for the compounds might be written $\text{Me}_2\text{O}_2 (\text{Me}'_{m-1} \text{R}_m \text{O}_{3m+1})$ where Me' is the 12 coordinated metal atom in the perovskite layers and R the 6 coordinated atom. The formulae for the above compounds, $\text{Bi}_2\text{O}_2(\text{CaNb}_2\text{O}_7)$, $\text{Bi}_2\text{O}_2(\text{Bi}_2\text{Ti}_3\text{O}_{10})$ and $\text{Bi}_2\text{O}_2[(\text{BaBi}_2)\text{Ti}_4\text{O}_{13}]$ thus have m values of 2, 3 and 4. The simplest case, $m=1$, would correspond to the formula $\text{Me}_2\text{O}_2(\text{RO}_4)$ and to a structure built up of Me_2O_2 layers and layers of RO_4 octahedra each octahedron sharing four corners. Compounds of this type have, however, not been successfully synthesized as yet.

The present paper deals with the compounds $\text{Bi}_2\text{NbO}_5\text{F}$, $\text{Bi}_2\text{TaO}_5\text{F}$ and $\text{Bi}_2\text{TiO}_4\text{F}_2$, which correspond to the simplest case, $m=1$ above, except that some of the O atoms are replaced by F atoms. The formulae of the compounds might thus be written: $\text{Bi}_2(\text{O}, \text{F})_2\text{Nb}(\text{O}, \text{F})_4$ etc.

Preparation, powder photographs and analyses

$\text{Bi}_2\text{NbO}_5\text{F}$: When a mixture of BiF_3 and Nb_2O_5 in the mol ratio 4:1 was heated in air at 800°C for a short time, a few single crystals (very thin plates) were obtained. Powder photographs of this sample indicated a tetragonal unit cell with the same cell dimensions as would be expected for the above general type when $m=1$. The best conditions for the formation of this phase were then studied by heating 2.5 g mixtures ($2\text{BiF}_3 + \frac{1}{2}\text{Nb}_2\text{O}_5$) in air at 640°C , this low temperature being chosen to reduce the volatility of the BiF_3 . The reaction times were varied from 5–40 hours, and powder photographs were taken of each product. For reaction times of 7–15 hours the lines of the above tetragonal phase predominated in the powder photographs, the few extra lines were very weak (see Table 1).

The fluorine content was found to vary from 4.0 % (7 hours) to 2.4 % (15 hours), whereas the calculated value for $\text{Bi}_2\text{NbO}_5\text{F}$ is 3.2 %. No variation in the size of the cell with the fluorine content was found, and it therefore seems probable that the composition of the phase is constant and that the observed variation in the F content is due to the presence of small impurities which are not visible in the powder photo-

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Table 1

Powder photographs of $\text{Bi}_2\text{NbO}_5\text{F}$ (sample with 2.8 % F)
Cr K radiation $\lambda_{\text{Cr K}\alpha} = 2.2909 \text{ \AA}$

hkl	$10^4 \cdot \sin^2 \theta_{\text{calc}}$	$10^4 \cdot \sin^2 \theta_{\text{obs}}$	I_{obs}
103	1319	1332	st
006	1708	1711	m
110	1784	1795	m
112	1974	1989	vw
105	2078	2083	vw
114	2543	2547	m
—	—	2785	vw
008	3036	3033	w
—	—	3093	vw
116	3492	3490	st
200	3568	3567	st
202	3758	3754	vw
—	—	3808	vw
{109	4734}	—	—
{00 10	4743}	4737	st
118	4820	4827	w
213	4888	4891	st
206	5276	5292	m
215	5647	5658	w
11 10	6527	6529	vw
10 11	6631	6630	w
00 12	6830	6841	w
220	7137	7139	w
222	7327	7330	vw
301	8076	8080	vw
{219	8303}	—	—
{20 10	8311}	8304	st
303	8456	8456	m
11 12	8614	8611	m
226	8845	8844	m
{10 13	8908}	—	—
{310	8921}	8919	m
312	9111	9119	vw
305	9215	9195	vw
00 14	9297	9292	vw

Fig. 1. C

Bi_2TiO_5
2:1 (total)
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phase are
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of $\text{Bi}_2\text{NbO}_5\text{F}$
 $\text{Bi}_2\text{TiO}_5\text{F}_2$

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graphs. To check that the Bi/Nb ratio had not changed essentially during the heating, a complete analysis was made on one sample (9 hours heating). The following values were obtained as the mean of three analyses: Bi: $68.0 \pm 0.6\%$, Nb: $14.2 \pm 0.6\%$, F: $3.7 \pm 0.2\%$.

The values calculated for $\text{Bi}_2\text{NbO}_5\text{F}$ are:

Bi: 68.5, Nb: 15.2%, F: 3.2%.

From these figures it seems probable that the formula of the compound is $\text{Bi}_2\text{NbO}_5\text{F}$.

$\text{Bi}_2\text{TaO}_5\text{F}$ was prepared in exactly the same way as $\text{Bi}_2\text{NbO}_5\text{F}$. No analysis was made since the powder photographs were similar to those of $\text{Bi}_2\text{NbO}_5\text{F}$ and niobium and tantalum compounds are usually isomorphous.

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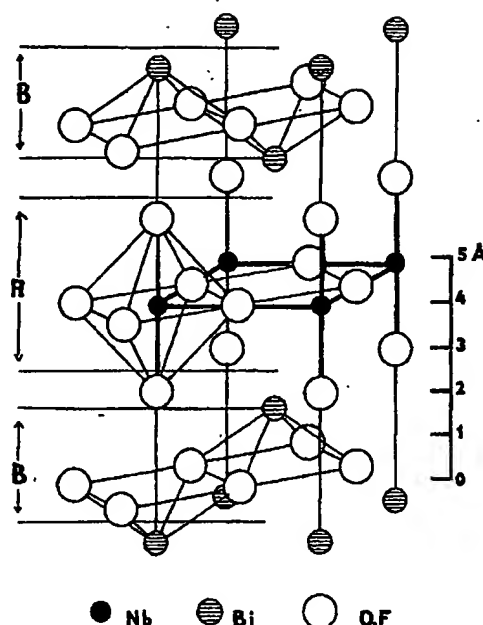


Fig. 1. One half of the unit cell of $\text{Bi}_2\text{NbO}_5\text{F}$. A denotes the region of $\text{Nb}(\text{O},\text{F})_6$ octahedra and B the $\text{Bi}_2(\text{O},\text{F})_2$ layers.

$\text{Bi}_2\text{TiO}_4\text{F}_2$: Mixtures of bismuth fluoride and titanium oxide in the mol ratio 2:1 (total 2.3 g) were heated in air at 640° for various lengths of time. The powder photographs obtained from samples heated for 3 or 5 hours could be interpreted by assuming a mixture of BiOF (2) and a phase whose cell dimensions were nearly the same as those of $\text{Bi}_2\text{NbO}_5\text{F}$. (See Table 2, where the reflexions from the BiOF phase are designated by b and those from the other phase by a). The fluorine contents of the mixed samples were found to be 6.4 % (5 hours) and 8.4 % (3 hours) but no variation of the cell size with the fluorine content was found. The calculated values are 7.8 % for BiOF and 6.7 % for $\text{Bi}_2\text{TiO}_4\text{F}_2$. From the original Bi/Ti ratio, from the fluorine analysis and from the similarity of the powder photographs with those of $\text{Bi}_2\text{NbO}_5\text{F}$ (Tables 1 and 2), it was concluded that the formula of the phase is $\text{Bi}_2\text{TiO}_4\text{F}_2$.

Methods of analysis: Fluorine. The samples were first decomposed by fusing with NaOH , and were then distilled with HClO_4 as described by WILLARD and WINTER (3). The distillate was titrated with $\text{Th}(\text{NO}_3)_4$ using Na-alizarinsulphonate as indicator.

Bismuth and Niobium. The samples were brought into solution, and niobium was determined as described in Scott's "Standard Methods" (4). Bismuth was first precipitated as Bi_2S_3 , which was then redissolved, converted to Bi_2O_3 and weighed as such.

Unit cells and space group

The dimensions of the unit cells were determined from powder photographs taken with focusing cameras of the Phragmén type (Tables 1 and 2). The radiation used

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Table 2

Powder photographs of $\text{Bi}_2\text{TiO}_4\text{F}_2$ (mixed with BiOF) Cr K radiation ($\lambda_{\text{Cr K}_\alpha} = 2.2909 \text{ \AA}$). a denotes the $\text{Bi}_2\text{TiO}_4\text{F}_2$ phase and b the BiOF phase

hkl	phase	$10^4 \sin^2 \theta_{\text{calc}}$	$10^4 \sin^2 \theta_{\text{obs}}$	I_{obs}
101	a	957	941	vvw
101	b	1270	1266	m
{103	a	1351	1354	st
{002	b	1352		
006	a	1771	1767	m
110	a	1816	1811	m
110	b	1864	1858	vvw
112	a	2013	1999	w
105	a	2138	2132	w ⁺
102	b	2284	2288	vvw
114	a	2603	2601	m
112	b	3216	3074	vw
107	a	3319	3231	w
116	a	3587	3320	vw
200	a	3631	3600	st
200	b	3728	3624	st
202	a	3828	3744	w
103	b	3974	3822	w
204	a	4418	3982	w
211	a	4538	4352	vvw
109	a	4893	4426	vvw
{113	b	4906	4590	w
{00 10	a	4919	4674	vvw
213	a	4982		
202	b	5080	4904	st
{206	a	5402	4979	st
{004	b	5408	5084	w
215	a	5769		
212	b	6012	5416	m ⁺
104	b	6340	5768	m
{203	b	6770	6025	m
{208	a	6779	6353	w
10 11	a	6860	6779	m
217	a	6950	6786	m
00 12	a	7084	6869	m
{220	a	7262	6950	vvw
{114	b	7272	7075	m
{220	b	7455	7262	m
{222	a	7459		
213	b	7702	7456	w
301	a	8210	7709	m
219	a	8524	8049	vw
{20 10	a	8550	8210	vw
303	a	8613	8352	vw
301	b	8736	8524	st
222	b	8814	8603	m
11 12	a	8900	8725	w
			8807	w
			8900	m

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Table 2 (continued)

hkl	phase	$10^4 \sin^2 \theta_{\text{calc}}$	$10^4 \sin^2 \theta_{\text{obs}}$	I_{obs}
2 2 6	<i>a</i>	9033	9027	m
3 1 0	<i>a</i>	9078	9072	w
2 0 4	<i>b</i>	9136	9136	vw
3 1 2	<i>a</i>	9275	9272	m
3 1 0	<i>b</i>	9319	9319	w
{ 1 0 5	<i>b</i>	9382 }	9384	m
{ 3 0 5	<i>a</i>	9400 }		

was $Cr K$ ($\lambda_{Cr K\alpha} = 2.2909 \text{ \AA}$). As mentioned above the powder photographs could be interpreted by assuming tetragonal unit cells; the cell dimensions are given below.

	a (Å)	c (Å)
$\text{Bi}_2\text{NbO}_5\text{F}$	3.835	16.63
$\text{Bi}_2\text{TaO}_5\text{F}$	3.829	16.64
$\text{Bi}_2\text{TiO}_4\text{F}_3$	3.802	16.33

The errors in these figures are estimated to be $\pm 0.1\%$.

The observed density was 8.0 for $\text{Bi}_2\text{NbO}_5\text{F}$ (preparation with 2.8% F), which agrees fairly well with the assumption of 2 formula units per unit cell, giving a calculated density of 8.26.

Zero and first order Weissenberg photographs around the a axis were taken. There was nothing in the Weissenberg photographs to indicate a Laue symmetry lower than $D_{4h} - 4/mmm$. The only extinctions found were that h, k, l were absent for $h+k+l$ odd, which is characteristic of the space groups C_{4v}^0 , D_{2d}^9 , D_{2d}^{11} and D_{4h}^{17} .

Powder photographs only were taken of the compounds $\text{Bi}_2\text{TaO}_5\text{F}$ and $\text{Bi}_2\text{TiO}_4\text{F}_3$, and from these it was concluded that these substances are isomorphous with $\text{Bi}_2\text{NbO}_5\text{F}$.

Positions of the metal atoms

$\text{Bi}_2\text{NbO}_5\text{F}$: With 2 formula units per unit cell there are 4 Bi and 2 Nb atoms per unit cell. The intensities of the spots in the Weissenberg photographs seemed in the main to depend only on the l values. Thus for l even $I_{001} \approx I_{111} \approx I_{201}$ etc. and for l odd: $I_{101} \approx I_{211} \approx I_{301}$ etc. With these intensity values a good approximation of the Patterson-Harker function along $00z$ could be obtained by using only the intensity values of $h0l$ and $h1l$. The Patterson-Harker function thus calculated (not given here) showed only one, big, maximum, at $z = 0.34$. This maximum, and the absence of others, could be explained only by assuming that 4 Bi atoms are situated at the positions $\pm 00z$ with $z = 0.17$ or $z = 0.33$, and the Nb atoms at the positions $00\frac{1}{2}$ or 000 . Arbitrarily choosing 000 as the position for Nb, trial and error calculations gave the value 0.325 for the Bi parameter.

No determination of z_{Bi} was made for $\text{Bi}_2\text{TaO}_5\text{F}$.

For $\text{Bi}_2\text{TiO}_4\text{F}_3$ the powder photograph data were used to determine the Bi parameter. Assuming the Ti atoms to be situated at 000 and the O and the F atoms to occupy the same positions as given below for $\text{Bi}_2\text{NbO}_5\text{F}$, the value $z_{\text{Bi}} = 0.327 \pm 0.006$ was obtained from trial and error calculations.

B. AURIVILLIUS, *The structure of $\text{Bi}_2\text{NbO}_5\text{F}$ and isomorphous compounds*Table 3
Weissenberg photographs of $\text{Bi}_2\text{NbO}_5\text{F}$

Zero layer

l	$h k$		0 0		2 0		4 0		l
			I_{calc}	I_{obs}	I_{calc}	I_{obs}	I_{calc}	I_{obs}	
0			—	—	170	vst	37	w	0
2			—	—	10	w	3	vw	2
4			0.3	—	0.04	—	0.05	—	4
6			220	vst	67	w	34	vw	6
8			12	w	5	vw	6	vw	8
10			3	vw	2	—	2	—	10
12			44	st	26	w	86	st	12
14			15	m	11	w			14
16			10	w	10	w			16
18			16	m	28	m			18
20			22	m					20

l	$h k$		1 0		3 0		l
			I_{calc}	I_{obs}	I_{calc}	I_{obs}	
1			7	w	1	vw	1
3			270	vst	42	w	3
5			40	w	8	vw	5
7			1	—	0.2	—	7
9			75	m	30	vw	9
11			18	w	10	vw	11
13			3	vw	3	vw	13
15			20	m	19	m	15
17			12	w			17
19			14	w			19

Positions of the O and the F atoms

The positions of the O and the F atoms could not be distinguished either from the diffraction data, or from space considerations because of the similarity in the reflecting power and ionic radii of O^{2-} and F^- . The problem is therefore treated as though O and F were the same atomic species. In the following, the O and the F atoms are denoted by (O, F) and the discussion relates to $\text{Bi}_2\text{NbO}_5\text{F}$ for which z_{Bi} could be accurately determined from the Weissenberg photographs.

It seemed reasonable to assume that the Nb atoms are surrounded by a regular or nearly regular octahedron of (O, F) atoms with distances $\text{Nb}-(\text{O, F}) \approx 2.0 \text{ \AA}$. Neglecting the polar space group C_{4v} , these conditions are fulfilled only if 4 (O, F) atoms, here called $(\text{O, F})_1$, are situated at the positions $\pm 00z$ with $z \approx 0.12$, and 4 (O, F) atoms, $(\text{O, F})_2$, at the positions $0\frac{1}{2}0, \frac{1}{2}00$. Assuming the distance (O, F)-(O, F) to be $\geq 2.5 \text{ \AA}$ and the distance $\text{Bi}-(\text{O, F})$ to be $\geq 2.2 \text{ \AA}$ there is only room for the remaining 4 (O, F) atoms, $(\text{O, F})_3$, at the positions $0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}$.

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Table
photographs of BiNbO_5F $\text{Cu K}\alpha$ radiation

First layer

4 0		$h k$		1 1		3 1	
I_{calc}	I_{obs}	l		I_{calc}	I_{obs}	I_{calc}	I_{obs}
37	w	0		210	vst	36	w
3	vw	2		17	w	4	vw
0.05	—	4		11	w	2	—
34	vw	6		110	m	33	w
6	vw	8		27	vw	9	vw
.....							
2	—	10		2	vw	1	—
		12		21	m	20	w
86	st	14		14	w	20	w
		16		5	w	17	w
		18		19	m		
		20		58	st		

$h k$		0 1		2 1		4 1	
l		I_{calc}	I_{obs}	I_{calc}	I_{obs}	I_{calc}	I_{obs}
1		7	—	2	vw	1	vw
3		270	vst	74	m	33	w
5		40	m	13	w	7	—
7		1	—	0.3	—	0.2	—
.....							
9		75	vst	40	w	53	w
11		18	m	12	vw	51	w
.....							
13		3	vw	3	vw		
15		20	m	19	m		
17		12	w	19	m		
19		14	w				

The coordination and distances in Å will be:

$$\begin{aligned}
 \text{Bi}-4 (\text{O}, \text{F})_3 &= 2.29 & \text{Nb}-2 (\text{O}, \text{F})_1 &= 2.0 \\
 \text{Bi}-4 (\text{O}, \text{F})_1 &= 2.9 & \text{Nb}-4 (\text{O}, \text{F})_2 &= 1.92 \\
 (\text{O}, \text{F})_3-4 (\text{O}, \text{F})_3 &= 2.71 & (\text{O}, \text{F})_2-4 (\text{O}, \text{F})_2 &= 2.71 \\
 (\text{O}, \text{F})_1-4 (\text{O}, \text{F})_3 &= 2.9 & (\text{O}, \text{F})_1-4 (\text{O}, \text{F})_2 &= 2.8
 \end{aligned}$$

The proposed structure is given in the summary. Calculated and observed intensities for the reflexions in the Weissenberg photographs are given in Table 3. I_{calc} is derived as follows:

$$I_{\text{calc}} = \frac{1 + \cos^2 2\theta}{1600 \cdot \sin 2\theta} \cdot F^2 \text{ where } F = \sum f \cos 2\pi(hx + ky + lz).$$

The lines of maximum absorption in the Weissenberg photographs (see 5) are indicated by dotted lines in Table 3. If the absorption effects are taken into account, the agreement between calculated and observed intensities is quite good.

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distance (O, F)–
is only room for

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Discussion of the structure

Even if the $(\text{O}, \text{F})_1$ atoms (see above) are assumed to occupy such a position that the distance $\text{Bi}-4(\text{O}, \text{F})_1$ is as small as possible [$z(\text{O}, \text{F})_1 = 0.15$, $(\text{O}, \text{F})_1 = 2.5$, $\text{Nb}-2(\text{O}, \text{F})_1 = 2.5$, $\text{Bi}-4(\text{O}, \text{F})_1 = 2.7$], the distance $\text{Bi}-4(\text{O}, \text{F})_1$ will still be much longer than the distance $\text{Bi}-4(\text{O}, \text{F})_3$. It therefore seems appropriate to describe the structure of $\text{Bi}_2\text{NbO}_5\text{F}$ as being built up of $\text{Bi}_2(\text{O}, \text{F})_2$ layers alternating with octahedral layers having the composition $\text{Nb}(\text{O}, \text{F})_4$, both layers being perpendicular to the c -axis. It might be pointed out that the structure of $\text{Bi}_2(\text{O}, \text{F})_2\text{Nb}(\text{O}, \text{F})_4$ is basically of the same type as the " X_1 structures", $\text{Me}_2\text{O}_2\text{X}$, previously investigated by SILLÉN (6). Thus the octahedral sheets $\text{Nb}(\text{O}, \text{F})_4$ correspond to single layers of halogen atoms, X , in $\text{Me}_2\text{O}_2\text{X}$.

Discussion of the distribution of the O and the F atoms

As seen above, the distance $\text{Bi}-4(\text{O}, \text{F})_3$ is 2.29 Å for $\text{Bi}_2\text{NbO}_5\text{F}$. For $\text{Bi}_2\text{TiO}_4\text{F}_2$ the corresponding distance is calculated to be 2.26 ± 0.06 Å. These distances are very nearly the same as the corresponding distances, $\text{Bi}-4\text{O}$, within the Bi_2O_7 layers of other bismuth oxicomounds (6). This need not, however, necessarily mean that the $\text{Bi}_2(\text{O}, \text{F})_2$ layers (see the figure) are free from F atoms, since compounds with $\text{Bi}_2(\text{O}, \text{F})_2$ layers which certainly contain F atoms have not been investigated hitherto, and thus the distances within such layers are unknown.

For the present it seems therefore best to make no special assumptions as to the distribution of the O and F atoms.

SUMMARY

The crystal structure of $\text{Bi}_2\text{NbO}_5\text{F}$ has been investigated by means of Weissenberg and powder photographs. From powder photographs the compounds $\text{Bi}_2\text{TaO}_5\text{F}$ and $\text{Bi}_2\text{TiO}_4\text{F}_2$ have been found to be isomorphous with $\text{Bi}_2\text{NbO}_5\text{F}$. The following structure is proposed for $\text{Bi}_2\text{NbO}_5\text{F}$:

$D_{4h}^{27}-I\ 4/mmm$		
$(000, \frac{1}{2}\frac{1}{2}\frac{1}{2}) +$		
2 Nb	in 2 (a) :	000
4 Bi	in 4 (e) :	$\pm 00z$
		$z = 0.325 \pm 0.001$
4 $(\text{O}, \text{F})_1$	in 4 (c) :	$0\frac{1}{2}0, \frac{1}{2}00$
4 $(\text{O}, \text{F})_2$	in 4 (e) :	$\pm 00z$
		$z = 0.12 \pm 0.01$
4 $(\text{O}, \text{F})_3$	in 4 (d) :	$0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}$

The cell dimensions are $a = 3.835$ Å, $c = 16.63$ Å for $\text{Bi}_2\text{NbO}_5\text{F}$. The positions of the metal atoms were determined from the diffraction data, those of the (O, F) atoms from space considerations. Although it does not seem improbable that O atoms alone occupy the positions $0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}$, Bi and O thus forming Bi_2O_7 layers as in other bismuth oxicomounds, nothing can be definitely stated as to the distribution of the O and F atoms.

The structure is built up of quadratic $\text{Bi}_2(\text{O}, \text{F})_2$ layers alternating with octahedral sheets having the composition $\text{Nb}(\text{O}, \text{F})_4$ (see figure) and the formula might thus be written: $\text{Bi}_2(\text{O}, \text{F})_2\text{Nb}(\text{O}, \text{F})_4$. The structure is formally related to a series of

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previously investigated structures of general formula $Me_2O_2 (Me'_{m-1}R_mO_{3m+1})$ and represents the simplest case of this series, i.e. $m=1$.

University of Stockholm, Institute of Inorganic and Physical Chemistry, May 1952.

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such a position
=0.15, (O, F)₁₋₄
3i-4 (O, F)₁ will
efore seems ap-
ip of Bi₂(O, F)₂
Nb (O, F)₄, both
at the structure
tures", Me_2O_2X
(O, F)₄ correspond

toms.

For Bi₂TiO₄F,
se distances are
within the Bi₂O₃
necessarily mean
ince compounds
een investigated

ptions as to the

of Weissenberg
s Bi₂TaO₅F and
following struc-

The positions of
e of the (O, F)
le that O atoms
Bi₂O₃ layers as
to the distribu-

with octahedral
ula might thus
l to a series of

Tryckt den 24 november 1952

Uppsala 1952. Almqvist & Wiksells Boktryckeri AB